

# The Application of a Modified Form of the $S_N$ Method to the Calculation of Swarm Parameters of Electrons in a Weakly Ionised Equilibrium Medium

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Received March 23, 1982

A numerical method is developed for the solution of the Boltzmann equation in order to calculate the swarm parameters of a weakly ionised gas. A brief description is given of the three main types of swarm experiment in which the measurements of these parameters are usually carried out. Then it is shown how these experiments can be simulated by calculation in order to explain the discrepancies observed between the parameters measured under the same conditions but in different experiments. A description is given of the present method of solution which uses both Lesaint's  $S_N$  method and an iterative process based on the so-called Eddington factor. The efficiency and the accuracy of this treatment is shown in two model cases which have already been investigated by several authors. It is observed that the number of iterations is drastically reduced and that the results obtained are of high accuracy.

## I. INTRODUCTION

Experimental determination of the transport parameters in a weakly ionised gas have been carried out for many years by means of swarm type experiments. At the present time, the measurements are so accurate that the values of the macroscopic quantities obtained allow (if compared to the transport parameters given by the microscopic calculations) the set of initial cross-sections to be modified and a new set to be constructed consistent with the measurements of the transport parameters [1]. This procedure has given very good results in the case of helium [2] and for many molecular gases such as nitrogen, oxygen, and carbon dioxide [3, 4].

To carry out this program many conditions must be fulfilled. First of all we must be sure that the microscopic study accurately simulates the experiment. It is now known that when the number of electrons in the system varies (i.e., when there is ionisation and attachment), the measured quantities are dependent on the mode of

observation [5, 6]. In this way, the measurements of the drift velocity and of the diffusion coefficients of electrons differ greatly according to the experiment (pulsed Townsend or time of flight, for example). More precisely, we can show that if the scattering gas is not electronegative, the drift velocity measured in the time of flight experiment is higher than the drift velocity measured in the pulsed Townsend experiment. We shall see later how the microscopic simulation of the main swarm experiments can be made in a simple way.

The calculation of cross sections will only be possible if the method of solution giving the electron distribution function is very accurate. There are two methods which allow the rigorous calculation of transport coefficients in a gas under an electric field: (1) the Monte Carlo simulation and (2) treatment by the Boltzmann equation.

The Monte Carlo simulation is nowadays very often used, but it usually involves excessive computing time. It cannot be applied to the determination of cross sections and it is mainly restricted to checking the accuracy of the assumptions made in the resolution of the Boltzmann equation.

For reasons of simplicity, most works based on the Boltzmann equation adopt the two-term expansion approximation of the distribution function. This assumption, which allows the determination of the isotropic part of the distribution function by the means of a second-order differential difference equation, is fully valid only when the ratio of the electric field  $E$  to the molecule density  $N$  is weak or when the action of inelastic collisions is smaller than that of elastic collisions. In the case of molecular gases, for example, the action of inelastic collisions (rotation or vibration) is important even though the value of the  $E/N$  ratio is low. The anisotropy of the distribution function is then very strong and the two-term expansion of the distribution function is no longer valid.

Some recent works have been devoted to the solution of the Boltzmann equation in order to develop new methods able to give the velocity distribution function of electrons whatever the value of the  $E/N$  ratio or the kind of scattering gas.

We shall see later that generally the simulation of swarm experiments only needs the solution of the Boltzmann equation in a hydrodynamic (i.e., equilibrium) regime [7] in which the distribution function depends only on the density of electrons and on their derivatives.

There are roughly four different ways to attack the solution of the Boltzmann equation in this case. First we may put the equation in its integral form and use an iterative process. This is the method developed by Rees [8] in the study of the transport of electrons in semi-conductors and by Kleban and Davis [9, 10] in the determination of the  $E/N$  variation of the drift velocity of electrons in methane. We can show [11] that the number of iterations which are necessary to reach convergence is related to the number of collisions which are necessary to reach the equilibrium state. As the number of collisions is proportional to the inverse of  $E/N$ , the number of iterations will increase as  $E/N$  decreases (this becomes untrue as  $E/N$  approaches zero, i.e., as the electrons are almost at rest).

The calculation of the velocity distribution function by the integral method needs,

for every value of the velocity  $\mathbf{v}$ , to take into account in the integral term the whole set of  $\mathbf{v}$  values between zero and infinity. The computation of this integral term is very time consuming. It follows that the integral method (under the form adopted by Kleban and Davis) is not very efficient.

The second way to attack the rigorous study of the Boltzmann equation is to expand the distribution function  $f(\mathbf{v})$  in a series of spherical harmonics. We obtain an infinite system of differential difference equations paired by their successive anisotropies. Using the Galerkin method and expanding into a series of  $B$ -spline functions, Pitchford [12] has been able to solve this system whatever the number of anisotropies considered. The distribution function  $f(\mathbf{v})$  is then obtained by solving a large linear system, where the main matrix is block tridiagonal, which involves the use of a powerful computer.

Another way to attack the resolution of the Boltzmann equation, starting from the differential system mentioned above, consists of expanding the successive anisotropies in a series of Sonine orthogonal polynomials with a Maxwellian weight function, the associated temperature being connected to the mean energy of the electrons. This method, called the moment method, originates from the works of Grad [13], Kihara [14], and Kumar [15]. It has been applied to the study of the motion of the electrons in a weakly ionised gas by Lin *et al.* [16], and it is primarily interesting because the main macroscopic quantities are easily related to the expansion coefficients in orthogonal polynomials.

Although all the preceding methods are very different, they theoretically allow the rigorous calculation of the distribution function  $f(\mathbf{v})$  whatever its degree of anisotropy and whatever the kind of collision (elastic, inelastic, or ionisation) coming to play in the discharge. However, at the present time none of the above methods have been applied, to our knowledge, to the microscopic study of the motion of electrons with ionisation or/and attachment. In this case, as we shall see later, the simulation of the swarm experiments involves the resolution of a nonlinear equation and consequently needs an iterative process. So the methods of Pitchford and Lin *et al.* would be difficult to adapt as they are not iterative in nature, unlike the integral method of Kleban and Davis.

Until now the ionisation and attachment processes have mainly been included in the two-term expansion approximations [6]. The only general studies taking into account the ionisation and/or attachment collisions are those of Kitamori *et al.* [17]. Contrary to the three works mentioned above, Kitamori's treatment starts from the initial integrodifferential form of the Boltzmann equation and uses a finite difference approximation on the three variables  $v, \theta, t$ , where  $v$  is the module of the velocity vector  $\mathbf{v}$ ,  $\theta$  the angle between  $-\mathbf{E}$  and  $\mathbf{v}$ , and  $t$  the time. It is then possible to study the change with time of the macroscopic parameters before they reach the equilibrium state. But the parameters measured in the swarm experiments only depend on the  $E/N$  ratio, and the study of their change with time is not absolutely necessary. The essential point is to obtain equilibrium values with a great accuracy and with the shortest computing time. We can show that, as for the integral method, the time taken by the system to reach equilibrium is inversely proportional to  $E/N$ . That the number

of iterations depends on  $E/N$  in the iterative methods described above causes major inconveniences.

Our aim in the present paper is to eliminate this drawback by adapting to this problem the iterative technique on the so-called Eddington factor (developed by Hummer and Rybicki [18] in radiative transfer theory) and connecting it with a method of finite elements constructed by Lesaint [19] (roughly equivalent to the classical  $S_N$  method [20]). We shall see that the number of iterations necessary to reach the equilibrium state is small (less than ten in the worst case) and almost independent of the  $E/N$  ratio.

In the second part of this paper, we shall briefly give the various forms of the Boltzmann equation which allow the simulation of the hydrodynamic region of the main swarm experiments. We shall then give a detailed description of our method of solution. Lastly, we shall demonstrate its effectiveness in the calculation of the drift velocity and mean energy of the electrons for two model gases which have already been studied in previous works [10, 12, 16, 21].

## II. MICROSCOPIC DESCRIPTION OF SWARM EXPERIMENTS

There are three main classes of swarm experiments: the steady state Townsend (SST), the pulsed Townsend (PT), and the time of flight (TOF) experiments. In the SST device, a steady stream of electrons passes from the cathode to the anode of a drift tube and the electron current at the anode is measured using an electrometer. Ionisation and attachment coefficients are obtained in this simple arrangement [22]. If the anode is split into annular segments, the lateral diffusion coefficient  $D_T$  may also be measured [1]. In the PT system our electron swarm is emitted from the cathode in the form of a short-duration pulse which drifts and diffuses through the drift tube. The resulting current at the anode is recorded as a function of time. The parameters usually obtained in the PT experiment are the drift velocity and the longitudinal diffusion coefficient  $D_L$ .

The TOF swarm experiment is the most involved of the three mentioned above. In this case the distribution is observed in space as well as in time. Practically, there are several versions of the TOF experiment going from the Bradbury–Nielsen shutter method [1] to the most recent one developed by Blevin *et al.* [23].

Before going further into the description of the microscopic simulation of the swarm experiments we must, first of all, briefly recall the Boltzmann equation formalism. We know that in the case of a weakly ionized gas the Boltzmann equation describing the microscopic state of electrons takes the form

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \gamma \cdot \nabla_v f = C[f(\mathbf{r}, \mathbf{v}, t)]. \quad (1)$$

Here we shall be only concerned with binary collisions of electrons with a background gas (of atoms or molecules of mass  $M$  and number density  $N$ ) at rest. In

Eq. (1),  $\gamma = e\mathbf{E}/m$  is the acceleration of the electric field  $\mathbf{E}$  and  $C[f(\mathbf{r}, \mathbf{v}, t)]$  is the general collision operator;  $\mathbf{r}$  is the electron position.

We may write  $C$  as the sum of two terms  $-v_T f$  ( $v_T$  being the total collision frequency) and  $J[f(\mathbf{r}, \mathbf{v}, t)]$ , where  $-v_T f \frac{d\mathbf{r}}{dt} \frac{d\mathbf{v}}{dt}$  gives the number of electrons leaving the element  $d\mathbf{r} d\mathbf{v}$  of the phase space and  $J[f] \frac{d\mathbf{r}}{dt} \frac{d\mathbf{v}}{dt}$  the number of electrons coming into  $d\mathbf{r} d\mathbf{v}$ , whatever the kind of collision considered. Then we have

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \gamma \cdot \nabla_{\mathbf{v}} f + v_T f - J[f] = 0 \quad (2)$$

with

$$\begin{aligned} J[f] &= J_{\text{el}}[f] + J_{\text{ex}}[f] + J_{\text{ion}}[f], \\ J_{\text{el}}[f] &= N v \sigma_m(v) \varphi_0(v) + N \frac{m}{M} \cdot \frac{1}{v^2} \cdot \frac{\partial}{\partial v} (v^4 \sigma_m \varphi_0(v)), \\ J_{\text{ex}}[f] &= N \sum_k \frac{v_k^2}{v} \sigma_k(v_k) \varphi_0(v_k), \\ J_{\text{ion}}[f] &= N \frac{1}{\Delta} \cdot \frac{v_{\text{ion},1}^2}{v} \cdot \sigma_{\text{ion}}(v_{\text{ion},1}) \varphi_0(v_{\text{ion},1}) + \dots \\ &\quad + N \frac{1}{1-\Delta} \cdot \frac{v_{\text{ion},2}^2}{v} \cdot \sigma_{\text{ion}}(v_{\text{ion},2}) \varphi_0(v_{\text{ion},2}); \\ \varphi_0(v) &= \frac{1}{2} \int_0^\pi d\theta \sin \theta f(v, \theta), \\ v_k^2 &= v^2 + (2/m) \varepsilon_k, \\ v_{\text{ion},1}^2 &= \frac{v^2}{\Delta} + \frac{2}{m} \varepsilon_{\text{ion}}; \quad v_{\text{ion},2}^2 = \frac{v^2}{1-\Delta} + \frac{2}{m} \varepsilon_{\text{ion}}. \end{aligned}$$

In the above relationships,  $\Delta/(1-\Delta)$  is the electron energy partition ratio after an ionisation collision,  $\varepsilon_k$  and  $\varepsilon_{\text{ion}}$  are, respectively, the excitation of level  $k$  and ionisation thresholds,  $\theta$  is the polar angle between  $-\mathbf{E}$  and  $\mathbf{v}$ . The total collision frequency  $v_T$  is equal to  $N v \sigma_T$ , where  $\sigma_T$  is the microscopic total cross section defined by the relation

$$\sigma_T = \sigma_m + \sigma_a + \sigma_{\text{ex}} + \sigma_{\text{ion}},$$

where  $\sigma_m$ ,  $\sigma_a$ ,  $\sigma_{\text{ex}}$ , and  $\sigma_{\text{ion}}$  are, respectively, the momentum transfer, attachment, excitation, and ionisation cross sections. We note that

$$\sigma_{\text{ex}} = \sum_k \sigma_k,$$

where  $\sigma_k$  is the cross section of the excitation of level  $k$ .

Here we assume that collisions in the center of the mass system are isotropic. It follows that the collision operator  $J[f]$  is only a function of the isotropic part  $\varphi_0$  of the distribution function.

The microscopic simulation of the SST experiment is usually restricted to the region in the drift tube where electrons are in equilibrium with the electric field. In that case the ionisation or attachment coefficients no longer depend upon the position  $\mathbf{r}$  and we may write

$$f(\mathbf{r}, \mathbf{v}) = n(\mathbf{r}) F_{\text{SST}}(\mathbf{v}), \quad (3)$$

where  $f(\mathbf{r}, \mathbf{v})$  is the stationary distribution function,  $n(\mathbf{r})$  the density of electrons, and  $F_{\text{SST}}(\mathbf{v})$  the SST velocity distribution function defined so that

$$\int \underline{d\mathbf{v}} f(\mathbf{r}, \mathbf{v}) = n(\mathbf{r}), \quad (4a)$$

$$\int \underline{d\mathbf{v}} F_{\text{SST}}(\mathbf{v}) = 1. \quad (4b)$$

By integrating Eq. (1) in time between zero and infinity and taking into account Eq. (3) and the continuity equation, i.e.,

$$\nabla_r n = (\mathbf{v}_{\text{SST}}/v_{\text{SST}})(\alpha - \eta)n \quad (5)$$

( $v_{\text{SST}}$  being the module of the electron drift velocity in the SST experiment,  $\alpha$  and  $\eta$  ionisation and attachment coefficients, respectively), we have then the SST Boltzmann equation

$$\gamma \cdot \nabla_v F_{\text{SST}} + \left( v_T + \mathbf{v} \cdot \frac{\mathbf{v}_{\text{SST}}}{v_{\text{SST}}} (\alpha - \eta) \right) F_{\text{SST}} - J[F_{\text{SST}}] = 0 \quad (6)$$

with

$$\alpha = N \int \underline{d\mathbf{v}} v \sigma_{\text{ion}} F_{\text{SST}}(\mathbf{v}) / v_{\text{SST}}, \quad (7a)$$

$$\eta = N \int \underline{d\mathbf{v}} v \sigma_a F_{\text{SST}}(\mathbf{v}) / v_{\text{SST}}, \quad (7b)$$

$$\mathbf{v}_{\text{SST}} = \int \underline{d\mathbf{v}} \mathbf{v} F_{\text{SST}}. \quad (7c)$$

Relationships (7) show that the inclusion of  $\alpha$  and  $\eta$  terms in (6) involves the nonlinearity of this equation and, consequently, an iterative approach.

The  $\alpha$  and  $\eta$  terms come from the initial diffusion operator of Eq. (2) and account for the modification of the number of electrons in the drift tube under the influence of ionisation and attachment.

In the case of the PT experiment we may proceed in the same way as for the SST one, but we integrate in the position space (assumed infinite) and obtain the equation for the PT distribution function

$$\boldsymbol{\gamma} \cdot \nabla_{\mathbf{v}} F_{PT} + (v_T + (v_{ion} - v_a)) F_{PT} - J[F_{PT}] = 0, \quad (8)$$

where we set

$$v_{ion} = N \int d\mathbf{v} v \sigma_{ion} F_{PT}(\mathbf{v}), \quad (9a)$$

$$v_a = N \int d\mathbf{v} v \sigma_a F_{PT}(\mathbf{v}), \quad (9b)$$

and  $v_{ion}$  and  $v_a$  are the macroscopic ionisation and attachment frequencies for the PT experiment.

When ionisation or/and attachment occur,  $F_{SST}$  and  $F_{PT}$  differ significantly [5]. The drift velocity  $\mathbf{v}_{PT}$  for the PT experiment is given by

$$\mathbf{v}_{PT} = \int d\mathbf{v} \mathbf{v} F_{PT}(\mathbf{v}). \quad (10)$$

The TOF experiment can be simulated if the time before observation is long enough to allow a large number of collisions. The electron population has then reached its hydrodynamic state and the distribution function  $f(\mathbf{r}, \mathbf{v}, t)$  becomes separable into position, time, and velocity variables and can be expanded in a series in powers of the spatial gradient of the number density  $n(\mathbf{r}, t)$ , i.e.,

$$f(\mathbf{r}, \mathbf{v}, t) = \sum_{l=0}^{\infty} \tilde{f}^{(l)}(\mathbf{v}) \hat{l}(-\nabla_{\mathbf{r}})^l n(\mathbf{r}, t), \quad (11)$$

where  $(\nabla)^l$  represents an  $l$ -fold outer product of the gradient operator with itself and  $\hat{l}$  indicates an  $l$ -fold inner product operation. The coefficients  $\tilde{f}^{(l)}(\mathbf{v})$  in the expansion above are only velocity dependent tensors of rank  $l$ . If we substitute the expansion of  $f$  given by (11) into Eq. (1), we obtain a system of equations for the successive tensors  $\tilde{f}^{(l)}(\mathbf{v})$  [12]:

$$\boldsymbol{\gamma} \cdot \nabla_{\mathbf{v}} f^{(0)}(\mathbf{v}) + \omega^{(0)} f^{(0)}(\mathbf{v}) - C[f^{(0)}(\mathbf{v})] = 0, \quad (12a)$$

$$\boldsymbol{\gamma} \cdot \nabla_{\mathbf{v}} \tilde{f}^{(l)}(\mathbf{v}) - \mathbf{v} \cdot \tilde{f}^{(l-1)}(\mathbf{v}) + \sum_{j=0}^l \tilde{\omega}^{(j)} \tilde{f}^{(l-j)}(\mathbf{v}) - C[\tilde{f}^{(l)}(\mathbf{v})] = 0. \quad (12b)$$

In the above equations we set

$$\tilde{\omega}^{(l)} = \int d\mathbf{v} \mathbf{v} \tilde{f}^{(l-1)} + \int d\mathbf{v} C[\tilde{f}^{(l)}] \quad (13)$$

with the normalization conditions

$$\int \underline{dv} f^{(0)}(\mathbf{v}) = 1, \quad (14a)$$

$$\int \underline{dv} \tilde{f}^{(l)}(\mathbf{v}) = 0, \quad l \geq 1. \quad (14b)$$

In the presence of ionisation and attachment processes, the last integral in (13) becomes

$$\begin{aligned} \int \underline{dv} C[\tilde{f}^{(l)}] &= N \left[ \int \underline{dv} v \sigma_{\text{ion}} \tilde{f}^{(l)} - \int \underline{dv} v \sigma_a \tilde{f}^{(l)} \right] \\ &= \tilde{v}_{\text{ion}}^{(l)} - \tilde{v}_a^{(l)}. \end{aligned} \quad (15)$$

The  $-\omega^{(0)}$  parameter is the reaction rate; the drift velocity is given by  $\omega^{(1)}$  and the diffusion tensor by  $\tilde{\omega}^{(2)}$ . These two latter coefficients can be related to the measured TOF quantities [23]. Their microscopic calculations are made by iteratively solving system (12) with  $l = 2$ .

Further information about the hydrodynamic regime and the foundation of its microscopic treatment will be found in the paper of Kumar *et al.* [15].

The brief description above shows that the three classical swarm experiments may be simulated by some nonlinear kinetic equations deduced from the general linear form of the Boltzmann equation. We can put all these equations in the same form

$$\boldsymbol{\gamma} \cdot \nabla_v \psi + \bar{v} \psi - \bar{J}[\psi] = 0, \quad (16)$$

where  $\bar{v}$  and  $\bar{J}[\psi]$  differ according to the kind of experiment investigated.

In Section III we develop a numerical method of solution for Eq. (16) above.

### III. FINITE ELEMENT SOLUTION OF EQ. (16)

If in Eq. (16) the  $\boldsymbol{\gamma} \cdot \nabla_v \psi$  operator is written in spherical coordinates (the velocity vector  $\mathbf{v}$  being replaced by the pair  $v, \mu$ , where  $\mu$  is the cosine of the angle between  $-\mathbf{E}$  and  $\mathbf{v}$ ), and if we make the change of variables

$$r = \sqrt{2mv},$$

we are brought to the following equation:

$$\mu \frac{\partial \psi}{\partial r} + \frac{1 - \mu^2}{r} \cdot \frac{\partial \psi}{\partial \mu} + \alpha_T(r) \psi - \bar{J}[\psi] = 0, \quad (17)$$



where

$$\begin{aligned} \alpha_T(r) &= r\sigma_T/(2E/N), \\ \bar{J}[\psi] &= \bar{J}_{e1}[\psi] + \bar{J}_{ex}[\psi], \\ \bar{J}_{e1}[\psi] &= \frac{r\sigma_m(r)}{2E/N} \varphi_0(r) + \frac{m}{M} \cdot \frac{1}{2(E/N)r^2} \cdot \frac{\partial}{\partial r} [r^4\sigma_m\varphi_0], \\ \bar{J}_{ex}[\psi] &= \frac{r_{ex}^2}{2(E/N)r} \sigma_{ex}(r_{ex}) \varphi_0(r_{ex}), \\ r_{ex}^2 &= r^2 + \bar{r}^2, \\ \bar{r}^2 &= 4\varepsilon_{ex}, \\ \varphi_0(r) &= \frac{1}{2} \int_{-1}^{+1} d\mu \psi(r, \mu). \end{aligned}$$

We have restricted our study here to conservative situations (i.e., where there is neither ionisation nor attachment) and we have assumed that there is only one inelastic process (vibration or excitation of optical levels). The  $r$  variable is the square root of energy and is expressed in  $\text{eV}^{1/2}$ ;  $E/N$  and  $\sigma_T$  ( $\sigma_m$  and  $\sigma_{ex}$ ) are expressed in  $\text{volt} \cdot \text{cm}^2$  and  $\text{cm}^2$ .

Equation (17) has the same form as the neutron transport or radiative transfer equation for a spherical medium. The main discrepancy lies in the collision operator  $\bar{J}[\psi]$ .

Many investigations have been devoted to the numerical solution of equations such as (17). Although many methods have been set up, the  $S_N$  method initiated by Carlson [24] is probably the most used in neutron transport theory and several codes exist in one- or multigroup approximations. The  $S_N$  method being iterative, the main drawback which must be overcome is the prohibitive number of iterations. This problem will be left to one side for the moment and we shall now briefly describe the  $S_N$  scheme used in this work.

Our scheme comes from Lesaint's work [19] and is based on a method of approximation by continuous finite elements. We must first write Eq. (17) in the conservative form:

$$\begin{aligned} H\psi &\equiv \mu \frac{\partial}{\partial r} (r^2\psi) + r \frac{\partial}{\partial \mu} [(1-\mu^2)\psi] \\ &+ \alpha_T r^2\psi - r^2\bar{J}[\psi] = 0. \end{aligned} \quad (18)$$

We shall solve (18) on the area  $D = R^* \times \Omega$ , where  $r \in R^* = ]0, R[$  and  $\mu \in \Omega = ]-1; +1[$  with the boundary conditions

$$\psi(R, \mu) = \xi, \quad \mu < 0, \quad (19a)$$

$$\psi(0, \mu) = \psi(0, -\mu). \quad (19b)$$

Range  $R^*$  is taken as finite for numerical computations;  $\xi$  is an arbitrary constant  $R$  is chosen large enough so that  $\psi(R, \mu)$  and consequently  $\xi$  can be assumed small (the value of  $R$  is fixed to satisfy the inequality  $R^2\psi(R, \mu) \leq 10^{-6}$ ,  $\psi$  being normalized) Note that relation (19a) involves spherical symmetry in  $\psi(R, \mu)$  for large values of  $R$  in the backward direction. This assumption, which is not realistic in a general way, can be made here due to the low value of  $\xi$  chosen and since the function  $\psi$  is normalized. Numerical checks show that the values of the macroscopic quantities are the same whatever the dependency of  $\xi$  on  $\mu$ . The only differences are in the high energy part of the distribution function but the weight of these values is negligible if  $R$  is taken large enough. The choice of Eq. (19a) is similar, in the case of radiative transfer, to that of a finite spherical atmosphere with a flux of photons entering it from outside.

If we introduce the moments  $\varphi_j$  of order  $j$ ,

$$\varphi_j(r) = \frac{1}{2} \int_{-1}^{+1} d\mu \mu^j \psi(r, \mu); \quad j = 0, 1, 2, \dots, \quad (20)$$

we are led, by integrating (18) respectively in  $\mu$  and  $r$ , to the following conservative relationships:

$$\frac{\partial}{\partial r} (r^2 \varphi_1) + \alpha_T r^2 \varphi_0 - \frac{1}{2} r^2 \int_{-1}^{+1} d\mu \bar{J}[\psi] = 0 \quad (21)$$

and

$$\begin{aligned} r_b^2 \varphi_1(r_b) - r_a^2 \varphi_1(r_a) + \int_{r_a}^{r_b} dr \alpha_T(r) r^2 \varphi_0(r) \\ - \frac{1}{2} \int_{r_a}^{r_b} \int_{-1}^{+1} dr d\mu r^2 \bar{J}[\psi] = 0. \end{aligned} \quad (22)$$

Relationships (21) and (22) account for the conservation of the flux in the range  $R^*$  and the  $[r_a, r_b] \times \Omega$  array, respectively.

The basic idea in the building of the discrete scheme is to find functional forms for  $\psi(r, \mu)$  so that they satisfy the discrete approximations of conservative relations (21) and (22). With this aim we first replace the dense ranges  $R^*$  and  $\Omega$  by the discrete ones  $\bar{R}^*$  and  $\bar{\Omega}$  so that

$$\bar{R}^* = \{0 = r_0 < r_1 < \dots < r_I = R\}, \quad (23a)$$

$$\bar{\Omega} = \{-1 = \mu_{-J} < \mu_{-J+1} < \dots < \mu_0 = 0 < \mu_1 < \dots < \mu_{J-1} < \mu_J = 1\}. \quad (23b)$$

The  $I$  and  $J$  integers are greater than one. It follows that the new set  $\bar{D} = \bar{R}^* \times \bar{\Omega}$  is split in rectangular areas  $A_{ij}$ , where

$$A_{ij} = [r_i, r_{i+1}] \times [\mu_j, \mu_{j+1}]. \quad (24)$$

We shall assume as usual that

$$\mu_{-j+1} = \mu_{j-1}.$$

In each area  $A_{ij}$  ( $0 \leq i \leq I-1; -J \leq j \leq J-1$ ) we define the coefficients  $\theta_{i+1/2}$  and  $\alpha_{j+1/2}$  so that

$$0 < \theta_{i+1/2}, \alpha_{j+1/2} < 1,$$

$$\alpha_{j+1/2} = 1 - \alpha_{-j-1/2},$$

and the centered values  $r_{i+1/2}$  and  $\mu_{j+1/2}$  such that

$$r_{i+1/2} = \theta_{i+1/2} r_{i+1} + (1 - \theta_{i+1/2}) r_i, \tag{25}$$

$$\mu_{j+1/2} = \alpha_{j+1/2} \mu_{j+1} + (1 - \alpha_{j+1/2}) \mu_j. \tag{26}$$

In every  $A_{ij}$ , the function  $\psi$  is approximated by the expression  $\bar{\psi} = a + br + c\mu$ , which is determined by its values at the points (Fig. 1)  $(i, j + \frac{1}{2})$ ,  $(i + 1, j + \frac{1}{2})$ ,  $(i + \frac{1}{2}, j)$ , and  $(i + \frac{1}{2}, j + 1)$  with the following relationships being verified:

$$\theta_{i+1/2} \bar{\psi}_{i+1, j+1/2} + (1 - \theta_{i+1/2}) \bar{\psi}_{i, j+1/2} = \bar{\psi}_{i+1/2, j+1/2}, \tag{27}$$

$$\alpha_{j+1/2} \bar{\psi}_{i+1/2, j+1} + (1 - \alpha_{j+1/2}) \bar{\psi}_{i+1/2, j} = \bar{\psi}_{i+1/2, j+1/2}. \tag{28}$$

We must then find a function  $\bar{\psi}$  which is continuous for all values of  $A_{ij}$  and such that

$$\int_{A_{ij}} dr d\mu H\psi = 0, \quad 0 \leq i \leq I-1, \quad -J \leq j \leq J-1, \tag{29}$$

$$\psi(R, \mu_{j+1/2}) = \xi, \quad \mu_{j+1/2} < 0. \tag{30}$$

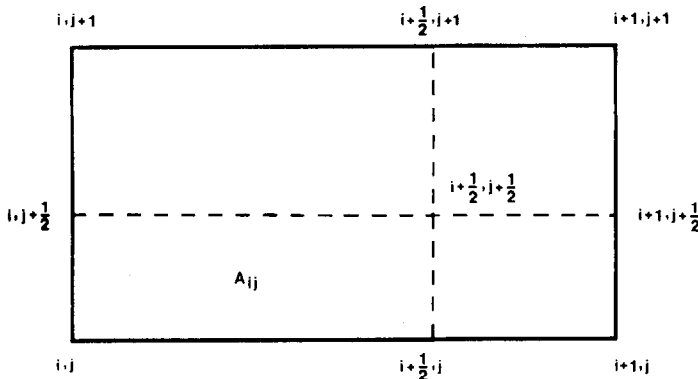


FIG. 1. Description of a cell in  $r - \mu$  space.

The numerical calculation of the quadratures in (29) is made with the two following relationships (where  $g_1$  and  $g_2$  are two arbitrary functions of  $\mu$  and  $r$ ):

$$\int_{\mu_j}^{\mu_{j+1}} d\mu g_1(\mu) \sim \omega_{j+1/2} g_1(\mu_{j+1/2}), \quad (31)$$

$$\int_{r_i}^{r_{i+1}} dr g_2(r) \sim w_{i+1/2} g_2(r_{i+1/2}). \quad (32)$$

In the discrete set  $\bar{D}$ , (29) may be written

$$w_{i+1/2} \omega_{j+1/2} H\bar{\psi}(r_{i+1/2}, \mu_{j+1/2}) = 0. \quad (33)$$

The variables  $r_{i+1/2}$  ( $0 \leq i \leq I-1$ ) and  $\mu_{j+1/2}$  ( $-J \leq j \leq J-1$ ) are defined by relations (25) and (26); the coefficients  $w_{i+1/2}$  and  $\omega_{j+1/2}$  are positive weights with the symmetry condition on  $\omega_{j+1/2}$

$$\omega_{j+1/2} = \omega_{-j-1/2}; \quad 0 \leq j \leq J-1. \quad (34)$$

The parameters  $\omega_{j+1/2}$ ,  $\omega_{-j-1/2}$ ,  $w_{i+1/2}$ , and  $r_{i+1/2}$  may be chosen in different ways. We make the approximate function  $\bar{\psi}$  verify discrete forms of conservative equations (21) and (22). By adding relations (33) for all  $j$  lying between  $-J$  and  $J-1$ , we see that the discrete form of relation (21) is satisfied if we have [19]

$$\sum_{j=-J}^{J-1} \omega_{j+1/2} \left( \frac{\partial}{\partial \mu} ((1-\mu^2) \bar{\psi}(r, \mu)) \right) (r_{i+1/2}, \mu_{j+1/2}) = 0, \quad 0 \leq i \leq I-1. \quad (35)$$

We then obtain the following conservative equation (discrete form of (21)):

$$\left[ \frac{\partial}{\partial r} (r^2 \bar{\varphi}_1) \right] (r_{i+1/2}) + \alpha_{T,i+1/2} r_{i+1/2}^2 \bar{\varphi}_0(r_{i+1/2}) - \frac{1}{2} r_{i+1/2}^2 \sum_{j=-J}^{J-1} \omega_{j+1/2} \bar{J}[\bar{\psi}_{i+1/2, j+1/2}] = 0, \quad (36)$$

where  $\bar{\varphi}_1$  and  $\bar{\varphi}_0$  are discrete approximations of  $\varphi_1$  and  $\varphi_0$ .

Substituting (28) in (35) produces

$$\begin{aligned} & \frac{\omega_{j+1/2}}{\mu_{j+1} - \mu_j} (1 + 2\mu_{j+1}\mu_{j+1/2} - 3\mu_{j+1/2}^2) \\ & = \frac{\omega_{j-1/2}}{\mu_j - \mu_{j-1}} (1 + 2\mu_{j-1}\mu_{j-1/2} - 3\mu_{j-1/2}^2) = \beta_j \end{aligned} \quad (37)$$

for  $-J + 1 \leq j \leq J - 1$  and

$$1 + 2\mu_{j-1}\mu_{j-1/2} - 3\mu_{j-1/2}^2 = 1 + 2\mu_{-j+1}\mu_{-j+1/2} - 3\mu_{-j+1/2}^2 = 0. \quad (38)$$

From the results above we can deduce the classical equality [20]

$$\beta_{j+1} - \beta_j = -2\mu_{j+1/2}\omega_{j+1/2}. \quad (39)$$

We may now add relations (36) for all  $i$  lying between  $I_1$  and  $I_2$ . To obtain the discrete form of (22), i.e.,

$$\begin{aligned} r_{I_2}^2 \bar{\varphi}_1(r_{I_2}) - r_{I_1}^2 \bar{\varphi}_1(r_{I_1}) + \sum_{i=I_2-1}^{i=I_1-1} w_{i+1/2} \alpha_{r,i+1/2} r_{i+1/2}^2 \varphi_0(r_{i+1/2}) \\ - \frac{1}{2} \sum_{i=I_2-1}^{i=I_1-1} \sum_{j=-J}^{j=J-1} w_{i+1/2} \omega_{j+1/2} r_{i+1/2}^2 \bar{J}[\bar{\psi}_{i+1/2,j+1/2}] = 0 \end{aligned} \quad (40)$$

we must set

$$r_{I_2}^2 \bar{\varphi}_1(r_{I_2}) - r_{I_1}^2 \bar{\varphi}_1(r_{I_1}) = \sum_{i=I_2-1}^{i=I_1-1} w_{i+1/2} \left( \frac{\partial}{\partial r} (r^2 \bar{\varphi}_1) \right) (r_{i+1/2}). \quad (41)$$

Since the function  $\psi(r, \mu)$  is linear for  $r$  and  $\mu$  in  $A_{ij}$ ,  $\bar{\varphi}_1$  is only linear with respect to  $r$ . It follows that relation (41) above must be verified in  $A_{ij}$  by the function  $\bar{\varphi}_1(r) = a' + b'r$  whatever the coefficients  $a'$  and  $b'$ . We then obtain the relations

$$r_{i+1}^2 - r_i^2 = 2w_{i+1/2}r_{i+1/2}, \quad 0 \leq i \leq I-1, \quad (42)$$

$$r_{i+1}^3 - r_i^3 = 3w_{i+1/2}r_{i+1/2}^2, \quad 0 \leq i \leq I-1. \quad (43)$$

Equations (42) and (43) allow the calculation of  $w_{i+1/2}$  and  $r_{i+1/2}$ . In order to obtain  $\omega_{j+1/2}$  and  $\mu_{j+1/2}$  from (37) and (38), we must add a supplementary relationship. To do that we observe (by using (37)), that if  $\omega_{j+1/2}$  is not very different from  $\mu_{j+1} - \mu_j$ , then  $\beta_j$  is almost equal to  $1 - \mu_j^2$ . For this reason we choose to set

$$\beta_j = 1 - \mu_j^2, \quad 0 \leq j \leq J. \quad (44)$$

Replacing  $\beta_j$  in (37) by the above value, we obtain the second-order equation

$$\begin{aligned} 3\mu_{j+1/2}^2(\mu_j^2 - \mu_{j+1}^2) + 2\mu_{j+1/2}(\mu_j - \mu_{j+1} - \mu_j^3 + \mu_{j+1}^3) \\ + \mu_{j+1}^2 - \mu_j^2 = 0, \end{aligned} \quad (45)$$

which gives us  $\mu_{j+1/2}$ . The weights  $\omega_{j+1/2}$  are then obtained by using (37) and the coefficients  $\theta_{i+1/2}$  and  $\alpha_{j+1/2}$  with the help of (25) and (26).

Taking into account the above relations (31)–(33) and (44), relation (33) may be written

$$\begin{aligned} &\omega_{j+1/2}\mu_{j+1/2}(r_{i+1}^2\bar{\psi}_{i+1,j+1/2} - r_i^2\bar{\psi}_{i,j+1/2}) \\ &+ w_{i+1/2}r_{i+1/2}(\beta_{j+1}\bar{\psi}_{i+1/2,j+1} - \beta_j\bar{\psi}_{i+1/2,j}) \\ &+ \omega_{j+1/2}w_{i+1/2}r_{i+1/2}^2(\alpha_{T,i+1/2}\bar{\psi}_{i+1/2,j+1/2} - \bar{J}[\bar{\psi}_{i+1/2,j+1/2}]) = 0. \end{aligned} \tag{46}$$

Using relations (25) and (26) we can write the above relation in the symmetrical form

$$\begin{aligned} &\bar{\psi}_{i+1/2,j+1/2}(\omega_{j+1/2}|\mu_{j+1/2}|A_{i+1/2}^- + w_{i+1/2}r_{i+1/2}B_{j+1/2} \\ &+ \omega_{j+1/2}w_{i+1/2}r_{i+1/2}^2\alpha_{T,i+1/2}) \\ &= \omega_{j+1/2}|\mu_{j+1/2}|A_{i+1/2}^-\bar{\psi}_{i+1,j+1/2} \\ &+ w_{i+1/2}r_{i+1/2}B_{j+1/2}\bar{\psi}_{i+1/2,j} \\ &+ \omega_{j+1/2}w_{i+1/2}r_{i+1/2}^2\bar{J}[\bar{\psi}_{i+1/2,j+1/2}] \end{aligned} \tag{47}$$

with  $I - 1 \geq i \geq 0$ ,  $-J \leq j \leq 0$ ; we set

$$B_{j+1/2} = (\alpha_{j+1/2}\beta_j + (1 - \alpha_{j+1/2})\beta_{j+1})/\alpha_{j+1/2}, \tag{48}$$

$$A_{i+1/2}^- = (r_i^2\theta_{i+1/2} + r_{i+1}^2(1 - \theta_{i+1/2}))/ (1 - \theta_{i+1/2}). \tag{49}$$

By  $|\mu_{j+1/2}|$  we denote the absolute value of  $\mu_{j+1/2}$ .

Equation (47) is only valid in the region where  $\mu_{j+1/2}$  is negative. If  $\mu_{j+1/2}$  is positive, we may use Eq. (47), but the  $A_{i+1/2}^-$  term must be replaced by  $A_{i+1/2}^+$  with

$$A_{i+1/2}^+ = (r_i^2\theta_{i+1/2} + r_{i+1}^2(1 - \theta_{i+1/2}))/\theta_{i+1/2} \tag{50}$$

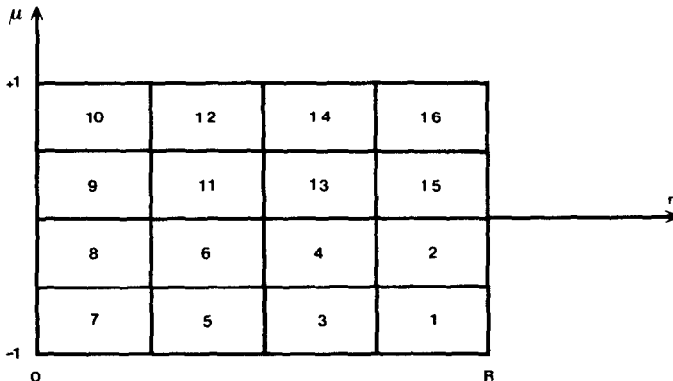


FIG. 2. Meshes in  $r - \mu$  space.

and  $\bar{\psi}_{i+1,j+1/2}$  by  $\bar{\psi}_{i,j+1/2}$ , with  $0 \leq i \leq I-1$ ,  $0 \leq j \leq J$ . When  $\mu$  equals  $-1$  ( $j = -J$ ), the derivative terms in  $\mu$  vanish and  $\bar{\psi}_{i+1/2,-j}$  is given by the equation

$$\begin{aligned} & \bar{\psi}_{i+1/2,-j} [A_{i+1/2}^- + w_{i+1/2} r_{i+1/2}^2 \alpha_{T,i+1/2}] \\ & = [A_{i+1/2}^- \bar{\psi}_{i+1,-j} + w_{i+1/2} r_{i+1/2}^2 \bar{J}[\bar{\psi}_{i+1/2,-j}]]. \end{aligned} \quad (51)$$

The determination of  $\bar{\psi}$  is carried out by means of Eqs. (42)–(51), (27), and (28). The iterative process is started with an arbitrary choice of  $\bar{\psi}$  allowing a first estimate of  $\bar{J}[\bar{\psi}]$ . The calculation of the successive  $\bar{J}[\bar{\psi}]$  values is made by using the values of  $\bar{\psi}$  obtained in the preceding iteration. The calculation follows the characteristic curves according to the scheme of Fig. 2.

#### IV. THE ACCELERATION PROCEDURE

By operating on (17) or (18) with

$$\frac{1}{2} \int_{-1}^{+1} d\mu \dots \quad \text{and} \quad \frac{1}{2} \int_{-1}^{+1} \mu d\mu \dots,$$

we obtain the two-moment equations

$$\frac{1}{r^2} \cdot \frac{\partial(r^2 \varphi_1)}{\partial r} = -\alpha_{\text{ex}}(r) \varphi_0(r) + \frac{1}{2E/N} \cdot \frac{m}{M} \cdot \frac{1}{r^2} \cdot \frac{\partial(r^4 \sigma_m \varphi_0)}{\partial r} + S_{\text{ex}}[\varphi_0(r_{\text{ex}})], \quad (52)$$

$$\frac{\partial}{\partial r} \varphi_2 = \frac{\varphi_0}{r} - 3 \frac{\varphi_2}{r} - \alpha_T \varphi_1. \quad (53)$$

We set

$$\alpha_{\text{ex}}(r) = \frac{r \sigma_{\text{ex}}(r)}{2E/N}, \quad (54)$$

$$S_{\text{ex}}[\varphi_0(r_{\text{ex}})] = \frac{r_{\text{ex}}^2}{r} \cdot \frac{\sigma_{\text{ex}}(r_{\text{ex}})}{2E/N} \cdot \varphi_0(r_{\text{ex}}), \quad (55)$$

$$r_{\text{ex}}^2 = r^2 + 4\varepsilon_{\text{ex}}.$$

The moments  $\varphi_l(r)$  have already been introduced above.

The system of equations (52) and (53) is not closed since it is a function of the three moments  $\varphi_0$ ,  $\varphi_1$ , and  $\varphi_2$ . In order to close it we may introduce in (52) and (53) the so-called Eddington factor  $f_{\text{ed}}(r)$  equal to the ratio  $\varphi_2/\varphi_0$  [18]. We obtain the new equations:

$$\frac{\partial K(r)}{\partial r} = \frac{1}{2E/N} \cdot \frac{m}{M} \cdot \frac{\partial}{\partial r} \left( r^4 \sigma_m \frac{H(r)}{f_{ed}(r)} \right) + r^2 \left\{ -\alpha_{ex} \frac{H(r)}{f_{ed}(r)} + S_{ex} \left[ \frac{H(r_{ex})}{f_{ed}(r_{ex})} \right] \right\}, \quad (56)$$

$$\frac{\partial H(r)}{\partial r} = \frac{1}{r} \left\{ H(r) \left( \frac{1}{f_{ed}(r)} - 3 \right) - \alpha_T \frac{K(r)}{r} \right\}, \quad (57)$$

where we set

$$K(r) = r^2 \varphi_1(r), \quad (58)$$

$$H(r) = f_{ed}(r) \varphi_0(r). \quad (59)$$

If the Eddington factor is known, Eqs. (56) and (57) allow the determination of the moments  $\varphi_0$  and  $\varphi_1$  (isotropic part and first anisotropy of the distribution function) taking into account the initial conditions generally unknown

$$K(R) = R^2 \varphi_1(R), \quad (60)$$

$$H(R) = f_{ed}(R) \varphi_0(R). \quad (61)$$

From the definition of  $f_{ed}$ , it can easily be seen that  $f_{ed}$  lies between  $\frac{1}{3}$  (when the distribution function is isotropic) and one (if all the electrons are in the forward direction). It follows that  $f_{ed}$  is a slowly varying function of  $r$  and that a rough approximation of  $f_{ed}$  in (56) and (57) will lead to a good estimate of  $\varphi_0$  and  $\varphi_1$ . Equations (56), (57), (60), and (61) can then be connected to Eqs. (47)–(51) and the Eddington factor  $f_{ed}$  may be obtained from the  $S_N$  calculations. We may then proceed as follows: First we choose an approximate value for  $f_{ed}$  ( $\frac{1}{3}$  for example) and we use it to solve (56) and (57) with some arbitrary initial conditions. The values of  $\varphi_0$  so obtained are normalized to one and put into  $\bar{J}[\bar{\psi}]$ . A new estimate of  $f_{ed}$  can be drawn up by using Eqs. (47)–(51). A new solution of (56) and (57) is made with the last estimate of  $f_{ed}$  and with the values of  $K(R)$  and  $H(R)$  coming from the  $S_N$  calculations. The process is then repeated until convergence.

The numerical solution of Eqs. (56) and (57) is straightforward and a Runge–Kutta scheme or a predictor–corrector method is very convenient.

The idea of iteration on the Eddington factor is not new, having previously been used in radiative transfer theory [25]. However, the use of the  $S_N$  method as a tool to calculate  $f_{ed}$  does not seem to have been adapted yet. Hummer and Rybicki [18], for example, obtain  $f_{ed}$  with the Fautrier method. They are led to the solution of a linear block tridiagonal system, the resolution of which is much more time consuming than the simple sweeping of the area  $\bar{D}$  which suffices in our case.



## V. NUMERICAL RESULTS

In order to check the effectiveness and the accuracy of our method, we have chosen two model situations which have already been investigated by Pitchford *et al.* [12], Braglia [21], Lin *et al.* [16], and Reid [26].

In the first model case the cross sections roughly approximate those of methane (Fig. 3). The synergism between the Ramsauer minimum in the momentum transfer cross section and the first vibrational process involves a large anisotropy in the distribution function [9] and makes this case very interesting to check the different methods.

In Table I we tabulate the number of iterations necessary to reach convergence with and without an accelerating process. The expression  $t/t_1$  is the ratio between the calculation times at  $E/N$  and at  $E/N = 1Td$ . The number of iterations and the calculation time become clearly independent of  $E/N$  when the acceleration process comes into play.

We note that the stop test on the drift velocity is equal to  $10^{-5}$  %. The magnitude of the test is not realistic in practice, but it has been chosen here in order to accurately follow the evolution of the macroscopic parameters toward convergence. Nevertheless, the decrease in the number of iterations is spectacular.

In Table II we compare results of Braglia (Monte Carlo) and Lin *et al.* (moment methods) with ours for the drift velocity and the mean energy of electrons. We can

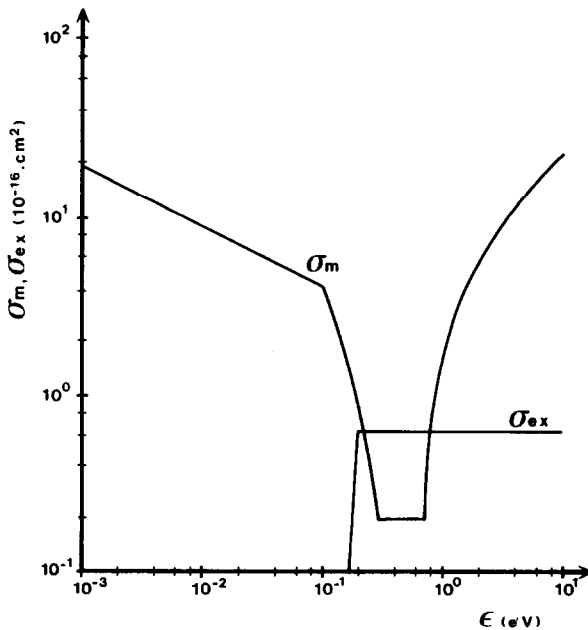


FIG. 3. Electron collision cross section in  $\text{CH}_4$  [21]:  $\sigma_m$ , momentum transfer;  $\sigma_{ex}$ , inelastic.

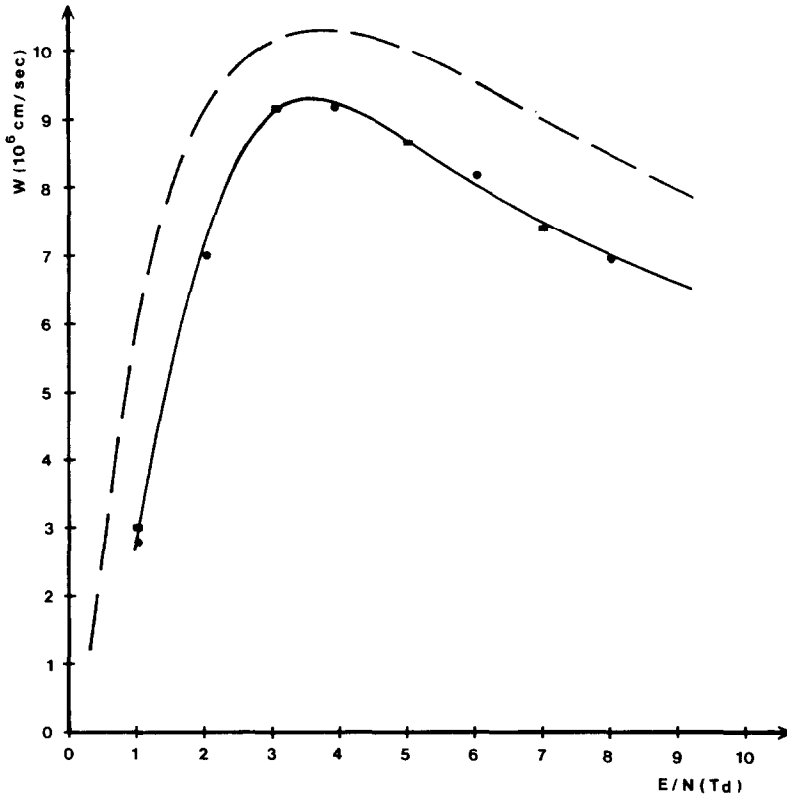


FIG. 4. Electron drift velocity as a function of  $E/N$ : solid curve, present work; circles, Monte Carlo simulation of Braglia [21]; squares, moment theory [16]. The dashed curve represents some experimental results.

TABLE I

Comparison of the Calculation Time ( $t$ ) with and without the Acceleration Process

$E/N$	With acceleration				Without acceleration			
	IT <sup>a</sup>	$t$	$t/t_1$	IT/IT <sub>1</sub>	IT	$t$	$t/t_1$	IT/IT <sub>1</sub>
1	IT <sub>1</sub> = 4	$t_1$ = 98.5	1	1	IT <sub>1</sub> = 30	$t_1$ = 487.2	1	1
2	6	150.2	1.5	1.52	87	1415.5	2.90	2.9
3	6	155.1	1.5	1.57	195	3180.1	6.53	6.5
3.9	8	205.2	2	2.08	354	5775.9	11.85	11.8
5	11	285.9	2.75	2.90	483	7891.7	16.20	16.1
6	7	182.2	1.75	1.85	636	10392	21.33	21.2
7	7	186.6	1.75	1.89	766	12508	25.67	25.53
8	7	176.4	1.75	1.79	923	15094	30.98	30.76
9	8	202.0	2	2.05				

<sup>a</sup> The number of iterations is given by IT.

TABLE II

Comparison of Present Results with Those of Braglia (Monte Carlo) and Lin *et al.* (Moments Method) in the Case of Methane

$E/N$ (Td)	Braglia		Lin <i>et al.</i>	Present work	
	$W$ ( $10^6$ cm/sec)	$\langle \epsilon \rangle$ (eV)	$W$ ( $10^6$ cm/sec)	$W$ ( $10^6$ cm/sec)	$\langle \epsilon \rangle$ (eV)
1	2.80	0.0759	3.07	2.88	0.0780
2	7.04	0.188	7.06	7.19	0.193
3.9	9.16	0.476	9.28	9.20	0.480
6	8.07	0.724	7.97	8.03	0.719
8	7.02	0.920	6.90	6.98	0.918

Note.  $W$  and  $\langle \epsilon \rangle$  are respectively the drift velocity and the mean energy of electrons.

TABLE III

Comparison of Our Results with Those of Pitchford (L.E.) and Reid (M.C.) in the Case of Model Gas for Several Values of  $2J + 1$

$E/N$ (Td)	$2J + 1$	$W$ ( $10^6$ cm/sec)
1	3	1.252
1	5	1.266
1	7	1.266
1	15	1.270
1	21	1.270
1	L.E. (7 terms)	1.272
1	M.C.	$1.255 \pm 0.013$
12	3	6.254
12	5	6.698
12	7	6.778
12	15	6.888
12	21	6.833
12	L.E. (7 terms)	6.839
12	M.C.	$6.87 \pm 0.069$
24	3	8.060
24	5	8.680
24	7	8.799
24	15	8.873
24	21	8.881
24	L.E. (7 terms)	8.883
24	M.C.	$8.890 \pm 0.089$

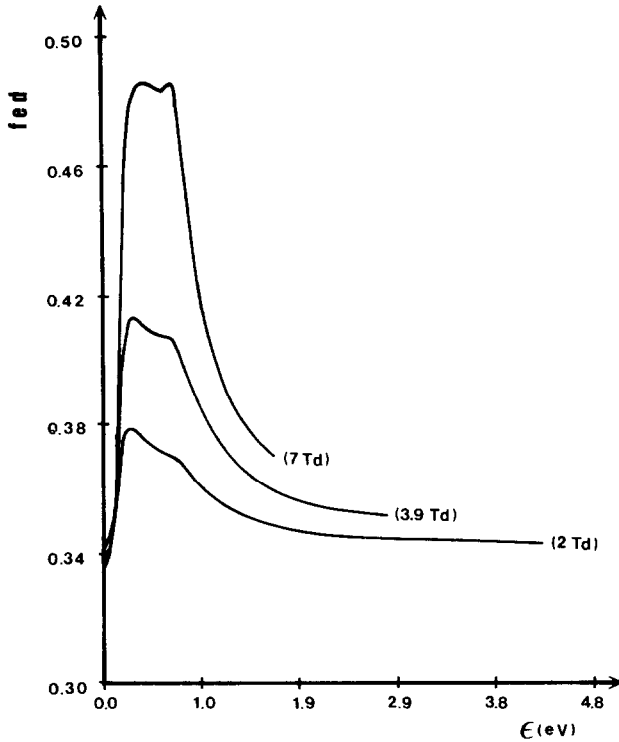


FIG. 5. Variation of the Eddington factor with energy for three values of  $E/N$ .

see the very good agreement between the overall results which verifies the accuracy of the different methods used. The corresponding curves are plotted in Fig. 4. The maximum in the drift velocity curve is connected with the increasing anisotropy of the distribution function. In Fig. 5 the variation of the Eddington factor is plotted against the electron energy for three different  $E/N$  values corresponding to the rising part, the maximum, and the decreasing part of the drift velocity, respectively. The Eddington factor deviates slightly from  $\frac{1}{3}$  and the largest value occurs in the minimum region of the momentum cross section.

The second case we deal with is the model atom of Reid [26]. His Monte Carlo results and those of Pitchford are available for comparison with our own. The momentum elastic transfer cross section is constant at  $6 \times 10^{-16} \text{ cm}^2$  and the inelastic cross section is of the form  $(10\epsilon - 2) 10^{-16} \text{ cm}^2$ , i.e., a ramp with a threshold energy at 0.2 eV. The neutral mass is 4 amu. Table III shows the drift velocity obtained with the three methods at three values of  $E/N$ . Our results compare well with both Monte Carlo and Pitchford values, providing a good check on the accuracy of our numerical method.

We note that in practice integers  $I$  and  $J$  were chosen as 151 and 7, respectively, in

the  $S_N$  calculations. Larger values involve a few changes in the macroscopic parameters and mainly affect the estimation of high order anisotropies of the distribution function.

## VI. CONCLUSION

In this work we have set up a numerical method of solution of the Boltzmann equation which can be applied to the calculation of the transport parameters measured in swarm type experiments. We have shown that, if we add to the Lesaint  $S_N$  method an accelerating process based on an iteration on Eddington factor, the number of iterations becomes very small and practically independent of the physical properties of the system ( $E/N$  value and type of background gas). Our results are in very good agreement with those obtained by other authors in the same physical situations.

Our feeling is that the method given in this paper is very likely to be one of the most powerful currently operating. Furthermore, it is very easy to set up and it may be run on quite a small computer. Whatever the type of background gas, the calculation of macroscopic quantities needs less than 128 K bytes in the central processor.

We restricted our investigations here to the situation where there is no ionisation or attachment in the swarm. But accounting for more involved processes is straightforward and currently we are running several programs quite satisfactorily for molecular gases ( $SF_6$ ,  $N_2$ ,  $O_2$ ,  $CH_4$ , etc.), allowing the calculation of the electron distribution function whatever the kind of collision occurring in the drift tube and whatever the strength of the anisotropy.

Most of the calculations in this paper were done on a SOLAR 16/65 minicomputer which is not very fast. To check the speed of our method, some runs have been carried out on an IBM 370 computer. In that case the calculation time is about one second. This time seems to be lower than the values given by Pitchford *et al.* corresponding to the same situation.

## REFERENCES

1. L. G. H. HUXLEY AND R. W. CROMPTON, "The Diffusion and Drift of Electrons in Gases," Wiley, New York, 1974.
2. R. W. CROMPTON, M. T. ELFORD, AND R. L. JORY, *Aust. J. Phys.* **20** (1967), 369.
3. A. G. ENGELHARDT AND A. V. PHELPS, *Phys. Rev.* **131** (1963), 2115.
4. R. D. HAKE AND A. V. PHELPS, *Phys. Rev.* **158** (1967), 70.
5. Y. SAKAI, H. TAGASHIRA, AND S. SAKAMOTO, *J. Phys. D* **10** (1977), 1035.
6. H. TAGASHIRA, Y. SAKAI, AND S. SAKAMOTO, *J. Phys. D* **10** (1977), 1051.
7. K. KUMAR, H. R. SKULLERUD, AND R. E. ROBSON, *Aust. J. Phys.* **33** (1980), 343.
8. H. D. REES, *J. Phys. Chem. Solids* **30** (1969), 643.
9. P. KLEBAN AND H. T. DAVIS, *Phys. Rev. Lett.* **39** (1977), 456.
10. P. KLEBAN AND H. T. DAVIS, *J. Chem. Phys.* **68** (1978), 2999.

11. G. L. BRAGLIA, *Beitr. Plasmaphys.* **12** (1980), 147.
12. L. C. PITCHFORD, S. V. ONEIL, AND J. R. RUMBLE, *Phys. Rev.* **23** (1981), 294.
13. H. GRAD, in "Handbuch der Physik," (S. Flügge, Ed.), Vol. 12, pp. 205–294, Springer-Verlag, Berlin, 1956.
14. T. KIHARA, *Rev. Mod. Phys.* **24** (1952), 45.
15. K. KUMAR AND R. E. ROBSON, *Aust. J. Phys.* **26** (1973), 157.
16. S. L. LIN, R. E. ROBSON, AND E. A. MASON, *J. Chem. Phys.* **71** (1979), 3483.
17. K. KITAMORI, H. TAGASHIRA, AND Y. SAKAI, *J. Phys. D* **13** (1980), 535.
18. D. G. HUMMER AND G. B. RYBICKI, *Mon. Not. R. Astron. Soc.* **152** (1971), 1.
19. P. LESAIN, "Sur la résolution des systèmes hyperboliques du premier ordre par des méthodes d'éléments finis," Rapport CEA-R-4731, Gif sur Yvette, 1976.
20. B. G. CARLSON, *Nucl. Sci. Eng.* **61** (1976), 408.
21. G. L. BRAGLIA, *J. Chem. Phys.* **74** (5) (1981), 2990.
22. V. N. MALLER AND M. S. NAIDU, *Proc. IEE* **123** (1976), 107.
23. H. A. BLEVIN, J. FLETCHER, AND S. R. HUNTER, *J. Phys. D* **11** (1978), 2295.
24. B. G. CARLSON, "Solution of the transport equation by  $S_N$  approximations," LA-1891, Los Alamos Scientific Laboratory, Los Alamos, N. Mex., 1955.
25. L. H. AUER AND D. MIHALAS, *Mon. Not. R. Astron. Soc.* **149** (1970), 65.
26. I. D. REID, *Aust. J. Phys.* **32** (1979), 331.